B-GROWTH

Gas bubble growth in decompressing magmas

USER MANUAL

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1. Introduction

This user manual describes the software B-Growth, which enables the user to calculate the evolution in time of a monodisperse population of gas bubbles in a magma undergoing a constant decompression. Among the assumptions made, two are particularly important. First, bubbles have all the same size and are assumed to be growing in place, without relative motion due to buoyancy. Rigorously, this means that the characteristic rise time (bubble diameter divided by the Stokes terminal velocity) should be much smaller than the decompression time scale. For most volcanological purposes, this translates into the fact that melt viscosity should not be too low (typically $>10^2$ Pa s). The second assumption is that the only volatile considered is water, the gaseous form of which is assumed to obey ideal gas law. This means that pressure should be kept between atmospheric to ~200 MPa.

The theory and further limitations of B-Growth are described in Forestier-Coste, L., Mancini, S., Burgisser, A., and James, F. (2012) *Numerical resolution of a monodisperse model of bubble growth in magmas*, Applied Mathematical Modelling, 36: 5936-5951 and Mancini, S., Forestier Coste, L., Burgisser, A., James, F., Castro, F. (2015) *An expansion-coalescence model to track gas bubble populations in magmas*, Bulletin of Volcanology. The physical basis of the bubble growth model is explained in the work of Lensky et al. (2004). Table 1 at the end of this user manual summarizes the variable symbols following the convention used in Mancini et al. (2015) and how they are referred to in the software and in the input/output files.

The source code is implemented in C++ using CodeLite 7.0 and wxWidgets through the wxCrafter interface embedded in CodeLite. A version compiled for Windows 7 (and compatible with Windows 8) is available at isterre.fr/annuaire/pages-web-du-personnel/alain-burgisser/article/softwares. Compilation for other systems (Linux, Mac) can be done by installing CodeLite on the desired system, loading the B-Growth.workspace file, and selecting Build/Run from the main menu. This creates an executable file in the B-GrowthWS/Release directory.

2. User interface description

We use here the nomenclature of Mancini et al. (2015), whereby a model run tracks the evolution in time, $\tilde{t}$, of the bubble radius, $\tilde{R}$ as a function of the ambient pressure $\tilde{P}_a$ (tilde indicate dimensional variables). Variables and their representation in the software are listed in Table 1.

The main window (Fig. 1) is separated into four horizontal panels: “Initial Values”, “Run Control”, “Run Parameters”, and “Output Control”.

The first panel (“Initial Values)” regroups the main physical variables and their initial values. The first series of variables are either set to their initial values (bubble radius, ambient pressure, and porosity), or are kept constant during the run (temperature, Henry’s constant, melt density, surface tension, and decompression rate). The decompression rate can be negative, in which case pressure increases until either of the minimum porosity, or the final pressure has been reached (see “Run Control” panel). Such compression runs are possible only with the “Simplified flux” and “Full” numerical schemes. The initial melt water concentration can be either set to a constant value manually, or set to the equilibrium value at the initial pressure using the solubility law by checking the “Equilibrium value” option.

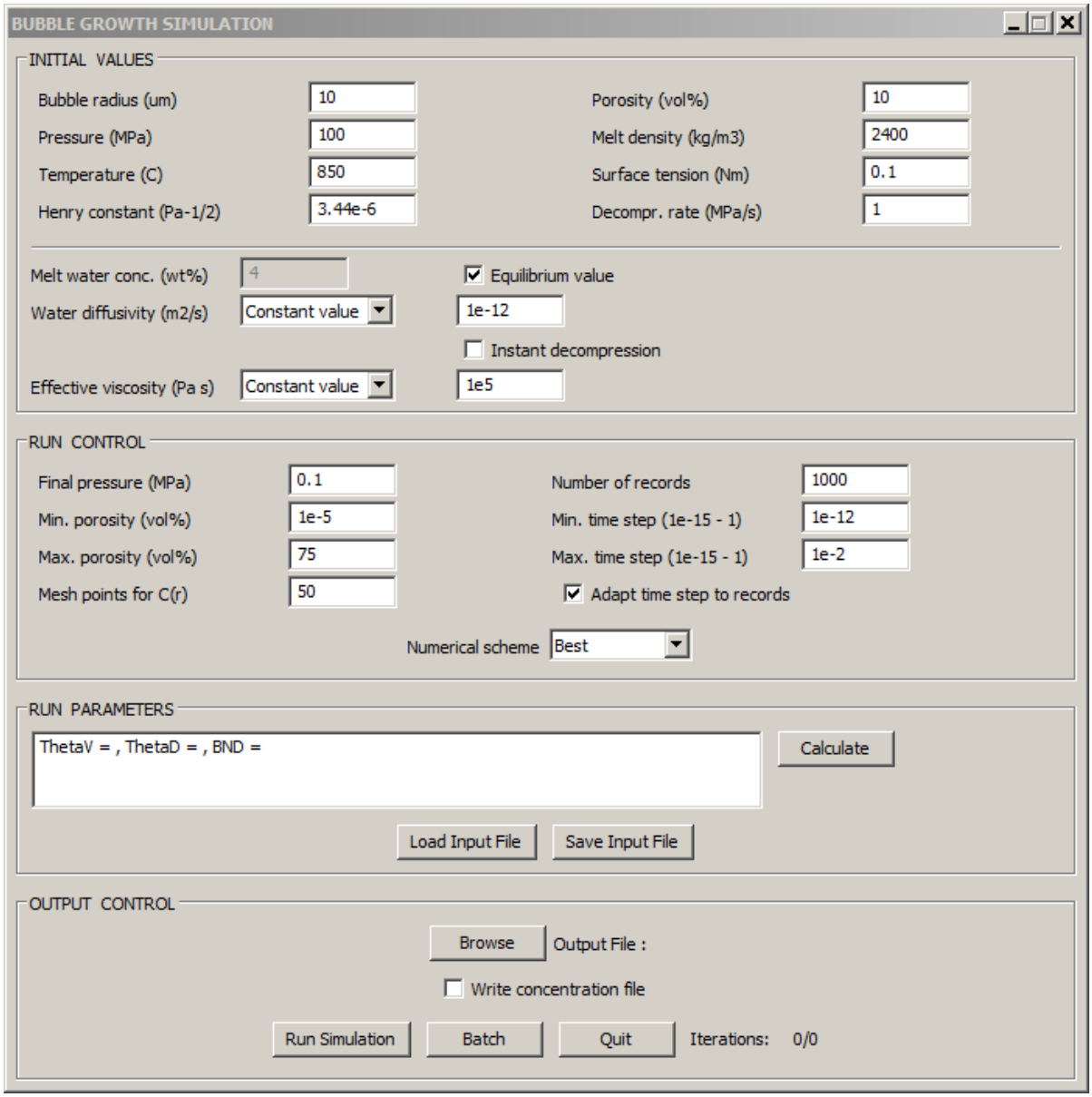

Figure 1: *Main window of B-Growth.*

The ambient pressure either changes linearly ("Instant decompression" unchecked), or instantly changes every time intervals set under "Time between jumps" ("Instant decompression" checked) so that the resulting series on pressure jumps approximates the linear decompression rate set under "Decompr. rate". The pressure jumps option cannot be set for compression runs (i.e. negative decompression rates).

Melt water content, C, can be calculated in two ways during a run. If the least number of assumptions is made, it varies as a function of the distance from the bubble edge ($\tilde{r}=\tilde{R}$) to the edge of the melt shell ($\tilde{r}=\tilde{S}$). Thanks to the solubility law, it is a function of ambient pressure at the bubble edge and its distribution within the melt shell is controlled by the advection-diffusion equation on $C(\tilde{t},\tilde{r})$. Hence, this first case implies that $C(\tilde{t},\tilde{r})=f(\tilde{P}_a,\tilde{r})$, which is abbreviated as f(P,r) in the software. In the second case, water content is assumed constant from bubble edge to melt shell edge, which can be calculated using the total water content (Mancini et al., 2015). Since is this case water concentration is updated at every step of the ambient pressure, $C(\tilde{t})=f(\tilde{P}_a)$, which is abbreviated as f(P) in the software. Note that some

numerical schemes (see "Run Control" panel) are assuming constant water content throughout the run and will ignore the setting "f(P,r)".

Water diffusivity can be set to 1) a constant value manually (option "Constant value"), 2) vary as a function of ambient pressure (option "f(P)"), which means that water content is constant from bubble edge to melt shell edge, or 3) vary as a function of ambient pressure and distance from bubble edge (option "f(P,r)"). In options 2) and 3), water diffusivity is calculated according to the melt type chosen under "Effective viscosity". In option 2), if the "Full" numerical scheme is selected, the water content for the diffusivity is calculated using the total water content. The relationships by Ni and Zhang (2008, Eq. 13) and Zhang and Ni (2010, Eq. 19) are used for rhyolite and phonolite, respectively. In the absence of current data on water diffusion in phonolitic melts but using the observation that melt SiO_2 content exerts stronger control on diffusion than alkali content (Zhang and Ni, 2010), phonolite diffusivity is assumed to be the same as that of a rhyolite. If no melt type has been chosen ("Constant value" under "Effective viscosity"), the relationship for rhyolite is assumed.

The effective viscosity can be set to 1) a constant value manually (option "Constant value"), 2) vary as a function of ambient pressure (options "f(P)"), which means that water content is constant from bubble edge to melt shell edge, or 3) vary as a function of ambient pressure and distance from bubble edge (options "f(P,r)"). In option 2), if the "Full" numerical scheme is selected, the water content for melt viscosity is calculated using the total water content. Melt viscosity can be either of rhyolitic (Hess and Dingwell, 1996), dacitic (Whittington et al., 2009), or phonolitic (Giordano et al., 2004). No consistency check is done between the run temperature ("Initial Values" panel) and the temperature range over which these relationships are valid.

The second panel ("Run Control") of the main window regroups variables affecting how a run is executed. The simulation stops when either the "Final pressure" value, or the "Max. porosity" value is reached, whichever occurs first. The run also stops when the "Min. porosity" value is reached, which may for instance occur if the melt water concentration is manually set to a value far from equilibrium at the initial ambient pressure (see the discussion on initial values in Forestier Coste et al., 2012, section 2.2). The number of points for the discretization of the distribution of the melt water concentration ("Mesh points of C(r)") is set to 50 by default, as it ensures relative errors $<10^{-3}$ on $\tilde{R}$, $\tilde{P}$, and α (Forestier Coste et al., 2012). The number of time steps recorded in the output file is set under "Number of records". Time steps vary according to the convergence criteria developed in Forestier Coste et al. (2012), except for the "Simplified flux" numerical scheme, which uses the smallest value between Eq. 32 and 33 of Forestier Coste et al. (2012) but also forces the change in time step from one iteration to the next to vary by a factor <2. The user can control this automatic adjustment by specifying minimum and maximum values ("Min. time step" and "Max. time step", respectively). Note that these values are dimensionless, which means that they are bounded between C++ standard precision ($\sim 10^{-15}$) and 1. They can be converted to dimensional times by multiplying them by $\tilde{P}_0/\Delta\tilde{P}$. This convention was chosen because it allows the user to estimate instantly how many time steps are needed to complete a run (e.g., $\delta t=10^{-8}$ means that $\sim 10^8$ iterations are needed to reach the final pressure). The option "Adapt time step to records" ensures that the run processes at least the number of time steps under "Number of records" so as to obtain a complete output file.

The "Numerical scheme" option allows the user to select how the system of equations is solved. The two dimensionless parameters Θ_D and Θ_V first proposed by Lensky et al. (2004) are used to characterize the different dynamical regimes of the equations system:

$$\Theta_D = \frac{\tilde{R}_0^2 \Delta\tilde{P}}{\tilde{D}_0 \tilde{P}_0} \qquad \text{and} \qquad \Theta_V = \frac{4\tilde{\eta}_{m0}\Delta\tilde{P}}{\tilde{P}_0^2}$$

The default option "Best" selects the most time-efficient scheme based on the values of Θ_D and Θ_V shown in Fig. 2. Options 1 to 8 force the software to use the corresponding limit cases shown in Fig. 2, which are described in Forestier Coste et al. (2012). The option "Simplified flux" uses

the approximation of the advection-diffusion equation described in Mancini et al. (2015). Finally, the option "Full" uses the generic resolution from Forestier Coste et al. (2012). These last two options accept negative decompression rates so as to simulate a compression of the magma.

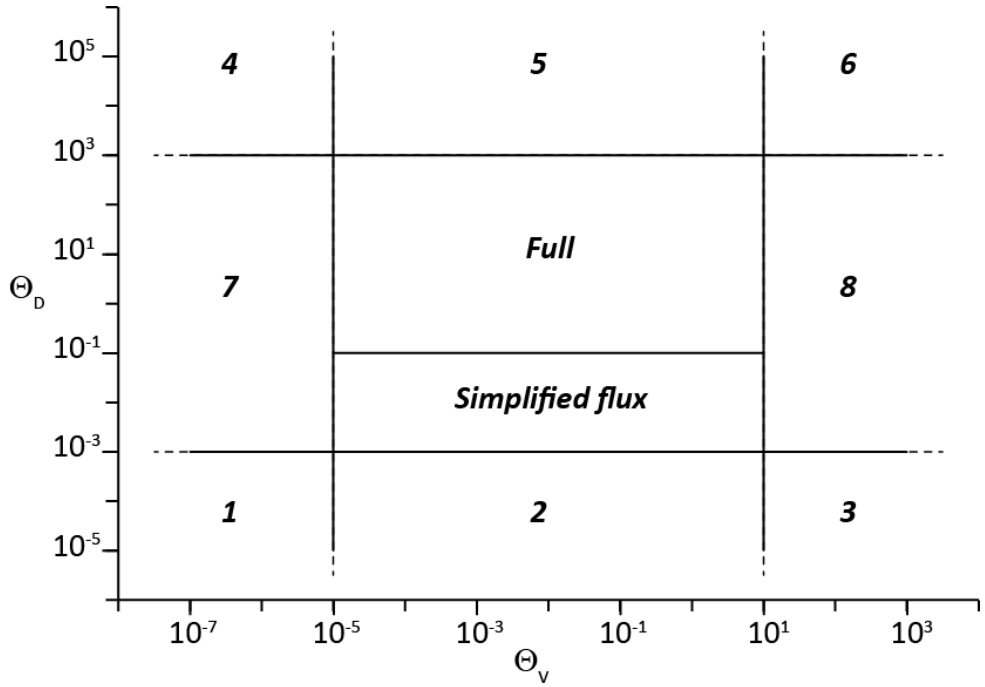

Figure 2: *Numerical schemes available in B-Growth as a function of the two dimensionless parameters Θ_D and Θ_V. See Mancini et al. (2015) for the implementation of the Simplified flux scheme and Forestier Coste et al. (2012) for the other schemes.*

The third panel ("Run Parameters") allows the user to calculate important additional parameters of the run. The "Calculate" button updates the two dimensionless numbers Θ_D ("ThetaD") and Θ_V ("ThetaV"), which characterize the dynamical regime of the run, the bubble number density with respect to the total volume ("BNDtot"), and the bubble number density with respect to the melt ("BNDmelt"). These four quantities are displayed with the numerical scheme in the text box on the left of the "Calculate" button. Initial values that the user has opted to calculate automatically (melt water concentration, water diffusivity, and effective viscosity) are also updated. The "Calculate" button tries to maintain some coherence among the various initial conditions selected, such as forcing the numerical scheme on "Full" or "Simplified flux" if a negative decompression rate is specified, but these cross checks are kept to a minimum (e.g., a run with a negative decompression rate but a final pressure lower than the initial pressure will be executed and presumably stop when the minimum porosity is reached, hence leaving the value of the final pressure unused). The user is thus the ultimate judge of the physical consistency of the run. Note that hitting the Enter key while editing any of the fields of the "Initial Values" and "Run Control" panels has the same effect as pressing the "Calculate" button.

The "Load Input File" and "Save Input File" buttons can be used to respectively read and write a text file that lists all the input and control parameters currently on display. The symbols used in the input file are listed in Table 1 (see the test file for syntax) and the file can be modified using a standard text editor to create series of input files for batch runs (see "Output Control" panel).

The fourth panel ("Output Control") allows the user to either run a single simulation, or a series of simulation in batch mode. A single simulation is run by first indicating the name of the output file using the "Browse" button. The symbols used in the tab-delimited output file are listed in Table 1. Checking the "Write concentration files" option will record two additional, tab-

delimited concentration files with the suffixes _c and _r added to the output file name. Each line of these two concentration files correspond to one time step of the output file. Each line of the _c file lists N values of melt water concentration $C(\tilde{r})$. Each line of the _r file lists N values of distance from the bubble edge $\tilde{r}$. Note that for schemes 1, 2, 6, and Simplified flux, N=1 in these files as C is constant across the melt shell. The "Run Simulation" button launches the single run and the current iteration number is updated at the bottom of the panel. A batch simulation is run by pressing the "Batch" button and selecting a text file that lists the full path and name of a series of input files that will be read and run sequentially (see the test file for syntax). Finally, the "Quit" button closes B-Growth.

3. Test files

Three input test files are provided (Rhyolite750.txt, Rhyolite850.txt, and Rhyolite950.txt). They can be loaded by using the "Load Input File" button (Fig. 1). Clicking successively on "Browse" to define an output file name and on "Run Simulation" should give outputs identical to those in the Rhyolite750_out.txt, Rhyolite850_out.txt, and Rhyolite950_out.txt files. Since the input file Rhyolite850.txt has the "Write concentration files" option checked, running it also produces the output files Rhyolite850_out_c.txt and Rhyolite850_out_r.txt.

The batch mode can be tested by clicking on "Batch" and selecting the BatchRhyolite.txt file, which will have for effect to generate automatically the 5 output files listed above. Be sure to first edit the BatchRhyolite.txt file and make sure that the 3 files listed there have the correct absolute path (e.g., C:\Users\My Name\B-Growth\Rhyolite750.txt).

4. References

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Hess, K-U., and Dingwell, D.B. (1996) Viscosities of hydrous leucogranitic melts: A non-Arrhenian model, American Mineralogist, v.81, p.1297-1300.

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Whittington, A.G., Hellwig, B.M., Behrens, H., Joachim, B., Stechern, A., and Vetere, F. (2009) The viscosity of hydrous dacitic liquids: implications for the rheology of evolving silicic magmas, Bulletin of Volcanology, v.71, p.185-199.

Zhang, Y., and Ni, H. (2010) Diffusion of H, C, and O components in silicate melts, Reviews in Mineralogy & Geochemistry, v.72, p.171-225.

Table 1: Meaning of variable names of the main window and the input/output files. Symbols in parenthesis are initial values.

Symbol	Main window	Input file	Output file	Variable
$4\pi\tilde{S}_0^3 C_T \tilde{\rho}_m/3$			WaterMass (kg)	Total water mass (kg)
C (C_0)	Melt water conc.	C_0 : ConcValue, EquConc	MeltWaterContent (wt%)	Melt water concentration
C_T				Total water concentration
$\tilde{D}$ ($\tilde{D}_0$)	Water diffusivity	$\tilde{D}_0$: DiffValue, Diff	Diffusivity (m^2/s)	Water diffusivity in melt (m^2/s)
$\tilde{G}_1$				H_2O molar mass (1.8×10^{-3} kg/mol)
$\tilde{G}_2$				Universal gas constant (8.3144 J/mol/K)
$\tilde{K}_H$	Henry constant	KHenry		Solubility constant ($Pa^{-½}$)
$\tilde{M}$ ($\tilde{M}_0$)				Scaled single bubble mass (kg), single bubble mass is $4\pi\tilde{M}/3$
N	Mesh points for C(r)	N	MeshPointsNb	Number of mesh points for melt water concentration
$\tilde{P}$			BubblePressure (MPa)	Bubble pressure (Pa)
$\tilde{P}_a$ ($\tilde{P}_0$)	$\tilde{P}_0$: Pressure, Final pressure	$\tilde{P}_0$: Pi, Pf	AmbientPressure (MPa)	Ambient pressure (Pa)
$\Delta\tilde{P}$	Decompr. rate, Time between jumps	DP, PStep, PStepValue	DecompressionRate (MPa/s)	Decompression rate (Pa/s)
$\tilde{r}$				Distance from bubble center (m)
$\tilde{R}$ ($\tilde{R}_0$)	Bubble radius	R0	Radius (μm)	Single bubble radius (m)
$\tilde{S}$ ($\tilde{S}_0$)				Influence zone radius (m)
$\tilde{t}$			Time (s)	Time (s)
δt	Max. time step, Min. time step	DtMin, DtMax	Dt	Time step (dimensionless)
$\tilde{T}$	Temperature	T	Temperature (°C)	Temperature (K)
α (α_0)	α_0 : Porosity, Max. porosity, Min. porosity	α_0 : Alpha, AlphaMax, AlphaMin	Porosity (vol%)	Porosity
$\tilde{\Sigma}$	Surface tension	Sigma	SurfaceTension (N m)	Surface tension (N m)
$\tilde{\eta}$	Effective viscosity	Visc	Viscosity (Pa s)	Effective magma viscosity (Pa s)
$\tilde{\eta}_m$ ($\tilde{\eta}_{m0}$)		$\tilde{\eta}_{m0}$: ViscValue		Melt viscosity (Pa s)
Θ_D	ThetaD		ThetaD	Diffusion parameter
Θ_V	ThetaV		ThetaV	Viscous parameter
$\tilde{\rho}_g$				Gas density (kg/m^3)
$\tilde{\rho}_m$	Melt density	Rhom	MeltDensity (kg/m^3)	Melt density (kg/m^3)
	BNDtot, BNDmelt			Bubble number densities (m^{-3})
	Number of records	NbRecords, ForceRecords		Number of time steps in output file
	Numerical scheme	Scheme		Numerical resolution method
		WriteConc		Flag indicating whether the concentration files are recorded